The spin-Peierls transition beyond the adiabatic approximation

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We develop a theory of the spin-Peierls transition taking into account the three dimensional character of the phonon field. Our approach does not rely on the adiabatic or mean field treatment for the phonons. It is instead based in the exact integration of the phonon field, the exact long wavelength solution of the one chain spin problem, and then a mean field approximation for the interchain interaction. We show that the spin gap and the critical temperature are strongly reduced due to the finite frequency effects of the phonon coupling transverse to the magnetic chains. We claim that our results should be applicable to the inorganic spin-Peierls compound $CuGeO_3$. We show that the long standing discussion on absence of a soft mode in this compound can be naturally resolved within our theory.

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I. INTRODUCTION

Quasi-one-dimensional electronic and magnetic materials are fascinating objects which have been intensively studied during the last decades. They show a variety of different phases as the magnetically dimerized, unconventional metal and triplet superconductor phases. It is possible to go from one phase to another by changing the experimentally accessible macroscopic parameters: pressure, temperature and the applied magnetic field. The different phases arise from the competition between the Coulomb repulsion between electrons and their coupling with the lattice degrees of freedom. Whereas the essential physics relies on the one-dimensionality of the electronic dynamics, the stabilization of the different phases depends on the three dimensional character of the system and thus on the interchain interaction. Transitions between the different phases are, in a way, a dimensional crossover from 1D to the three dimensionality of any real material.

Spin-Peierls systems are probably the simplest example of quasi-one-dimensional materials. They show a high temperature phase which can be well modelled by a one dimensional antiferromagnetic Heisenberg chain and a low temperature phase with lattice dimerization and spin singlet ground state. The transition between them arises from the competition between the gain in antiferromagnetic energy and the loss in elastic energy. It is indeed possible due to the three dimensional character of the phonon field. It is therefore very attractive to carefully understand the precise character of this transition as a representative of a large class of quasi-one-dimensional materials.

The theory of spin-Peierls (SP) transition was developed in the 1970's in connection with organic quasi-one-dimensional materials. The seminal work of Cross and Fisher[1] (CF) is nowadays taken as the canonical theory of the spin-Peierls transitions. It is based on a RPA approximation for the phonon field, which corresponds to neglecting the dynamics of the phonons. Otherwise the low energy spin correlations are exactly taken into account by the bosonization method. The CF theory is expected to work when the phonon frequency is much smaller than the spin gap. Moreover, CF have shown that corrections to RPA are small if the bare phonon frequency in the direction of the magnetic chain is much smaller than the phonon frequency perpendicular to the chains, that is to say if there is a *preexisting soft mode* before coupling phonons with the magnetism.

In this context the discovery of the first inorganic SP compound $CuGeO_3$ opened the possibility to experimentally study the dimerized phase and the phase transition with unprecedented precision[2]. The recent characterization of a new family of spin-Peierls materials with an incommensurate intermediate phase has renewed the interest on a precise description of the phase transition[3]. The picture that emerges from neutron scattering measurement of the phonon spectra in $CuGeO_3$ is the following[4,5]: at room temperature, there are two phonon modes relevant for the SP transition with $\omega_1 = 3.12\,THz$ and $\omega_2 = 6.53\,THz$ at the (0.5 0 0.5) point of the Brillouin zone. The phonon dispersion transverse to the propagation vectors of these relevant phonons is rather flat[5]. Therefore, *no preexisting soft* mode is observed and the RPA is not a priori justified. Moreover, on lowering the temperature, ω_1 and ω_2 do

not soften at the SP transition, as expected in the CF scenario. This is a strange behavior for a displacive structural phase transition.

On the other hand, Gros and Werner[6] (GW) have identified a parameter regime where the CF approach does not predict a softening of the relevant phonons but instead the appearance of a central peak in the dynamical structure factor at the transition point. The temperature dependence of the Peierls active phonon modes predicted by this analysis are in agreement with neutron scattering determinations in $CuGeO_3$. However the applicability of the adiabatic approximation or RPA in this material is not a priori justified.

In fact, what is missing for a complete understanding of the spin-Peierls transition in $CuGeO_3$, and possibly in other inorganic quasi-one-dimensional materials, is a theory which does not rely on the static approximation for the phonons. A first step in this direction was presented in [12], where the dynamics of the transverse phonons in the antiadiadatic limit was taken into account and the relevance the three dimensional character of the phonons was first brought to light. We give some more elements of such a theory in the present work.

The plan of the paper is as follows. In Section II, we start from a one-dimensional magnetic model coupled to two dimensional phonons and integrate out the phonon coordinates. Then we treat the effective in-chain interaction exactly by bosonization, and the inter-chain interaction by a mean field approximation. In Section III exact results for the 1D sine-Gordon model[7] are used to solve the mean field equations. By comparing with the adiabatic approximation we identify the relevant parameter to analyze the deviations from the adiabatic limit, namely the ratio between the frequency of phonon relevant for the SP transition ($\omega_\parallel$) and the frequency of the phonons transverse to the magnetic chain ($\omega_\perp$). The adiabatic limit is obtained only for high enough value of $\frac{\omega_\perp}{\omega_\parallel}$. Reducing this parameter both the gap and the spin-Peierls temperature are reduced. For $\omega_\perp \to 0$, *i.e.* the pure one dimensional problem, the gap and the SP temperature vanish. We discuss our results in connection with a recent study of the AF chain coupled to one-dimensional phonons[8]. In Section IV we study the dynamics of the SP relevant phonon mode in the high temperature phase, using a RPA on the effective interchain coupling generated by the spin-phonon interaction. We then address the question of absence of softening close to the SP transition. Finally, in Section V we present our conclusions and prospects for future related work.

II. THE EFFECTIVE INTERACTIONS INDUCED BY PHONONS

Let us start by considering a two dimensional system of spin $S = 1/2$ antiferromagnetic Heisenberg chains, with exchange constant $J_\parallel$ along one of the axes of a non-deformed square elastic lattice. We label by j chains, and by i the sites on each chain. The spin-phonon Hamiltonian is given by[9]:

$$H = \sum_{i,j} \frac{(P_i^j)^2}{2m} + \frac{1}{2} K_\parallel \sum_{i,j} (u_{i+1}^j - u_i^j)^2 + \frac{1}{2} K_\perp \sum_{i,j} \left((u_i^{j+1} - u_i^j)^2 \right) + J_\parallel \sum_{i,j} \left(1 + \alpha(u_{i+1}^j - u_i^j) \right) \vec{S}_i^j \cdot \vec{S}_{i+1}^j, \quad (1)$$

where u_i^j are the relevant (scalar) coordinates for ion displacements with respect to equilibrium positions, P_i^j are their conjugate momenta, $K_\parallel$ and $K_\perp$ are the elastic couplings along in-chain and inter-chain ions, respectively, and α measures the deformation effect on the magnetic exchange constants.

In the absence of phonons, we can write the bosonized low energy (long distance along the chains) Hamiltonian for the Heisenberg spin chains[10] as

$$H_{spin}^j = J_\parallel \sum_{i,j} \vec{S}_i^j \cdot \vec{S}_{i+1}^j \sim \frac{v_F}{2} \int dx \left(K_L \left(\partial_x \tilde{\phi}^j(x) \right)^2 + \frac{1}{K_L} \left(\partial_x \phi^j(x) \right)^2 \right), \quad (2)$$

where $x = ia$ (a being the lattice spacing), $\tilde{\phi}^j$ are the fields dual to the scalar fields ϕ^j, defined in terms of their canonical momentum as $\partial_x \tilde{\phi}^j = \Pi^j$, and : : stands for normal order with respect to the isolated chains ground state. The Fermi velocity of left and right excitations and the usual Luttinger parameter K_L depend on the XXZ anisotropy parameter, taking the values $v_F = \frac{\pi}{2} J_\parallel a$ and $K_L = 1$ for the isotropic Heisenberg chain with only nearest neighbor interaction. A marginal term $\lambda : \cos(2\sqrt{2\pi}\phi(x)) :$ has been discarded in eq.(2).

The term coupling spins with phonons can be treated perturbatively by using the continuum expression for the spin energy density

$$\vec{S}_i^j \cdot \vec{S}_{i+1}^j \sim \rho^j(x) = \frac{1}{\sqrt{2\pi}} \partial_x \phi^j(x) + (-1)^i \beta : \cos(\sqrt{2\pi}\phi^j(x)) : + \cdots \quad (3)$$

where β is a non-universal constant and the ellipses indicate higher harmonics[11]. Notice that : $\cos(\sqrt{2\pi}\phi^j)$: is a relevant operator of scaling dimension $D = 1/2$.

We will also assume that each chain dimerizes in such a way that the distortions can be approximately described as $u_i^j \approx (-1)^i u^j(x)$. Notice however that neighboring chains are not correlated *a priori*. Then

$$u_{i+1}^j - u_i^j \approx (-1)^{i+1}(2u^j(x) + a\partial_x u^j(x)). \tag{4}$$

We will keep only the leading order in the gradient expansion. The interaction Hamiltonian, in the continuum limit and up to leading order in the lattice spacing, then reads

$$H_{int} = \alpha J_{\parallel} \sum_{i,j}(u_{i+1}^j - u_i^j)\, \vec{S}_i^j \cdot \vec{S}_{i+1}^j = -g\sum_j \int dx\, u^j(x) \; : \cos(\sqrt{2\pi}\phi^j(x)): , \tag{5}$$

where $g \sim \frac{2\alpha J_{\parallel}\beta}{a}$.

Regarding the phonon Hamiltonian, we find it convenient to first construct the corresponding Lagrangian. Up to leading order in the lattice spacing the phonon Lagrangian can be written in the continuum limit as

$$L_{ph} = \frac{m}{2a}\sum_j \int dx \left[(\partial_t u^j(x,t))^2 - (\omega_{\parallel}^2 + \frac{1}{2}\omega_{\perp}^2)(u^j(x,t))^2 + \frac{1}{2}\omega_{\perp}^2 u^j(x,t)u^{j+1}(x,t) \right], \tag{6}$$

where $\omega_{\parallel}^2 = 4\frac{K_{\parallel}}{m}$ and $\omega_{\perp}^2 = 4\frac{K_{\perp}}{m}$.

Now we can write the action for the complete system and perform the usual Wick rotation $\tau = it$, arriving to the Euclidean action describing the low energy physics at finite temperature T:

$$
\begin{aligned}
S_E &= \sum_j S_{spin}[\phi^j] \\
&+ \frac{m}{2a}\sum_j \int dx\, d\tau \left((\partial_\tau u^j(x,\tau))^2 + (\omega_{\parallel}^2 + \frac{1}{2}\omega_{\perp}^2)(u^j(x,\tau))^2 - \frac{1}{2}\omega_{\perp}^2 u^{j+1}(x,\tau)u^j(x,\tau) \right) \\
&- g\sum_j \int dx\, d\tau\, u^j(x,\tau) \; : \cos(\sqrt{2\pi}\phi^j(x,\tau)): ,
\end{aligned}
\tag{7}
$$

where j runs from 1 to N, x from 0 to L, τ from 0 to $\beta = 1/T$, and the spin Euclidean action reads

$$S_{spin}[\phi^j] = \frac{1}{2}\int dx\, d\tau \left(\frac{1}{v_F}(\partial_\tau\phi^j(x,\tau))^2 + v_F(\partial_x\phi^j(x,\tau))^2 \right). \tag{8}$$

After Fourier transforming $j \to q$ (the wave vector perpendicular to the magnetic chains) , $\tau \to \omega_n$, with $\omega_n = \frac{2\pi n}{\beta}$ the Matsubara frequency, the phonon Green's function reads:

$$
\begin{aligned}
G^{jj'}(\tau,\tau') &= \frac{a}{m}\frac{1}{\beta}\sum_n \int_{-\pi}^{\pi} \frac{dq}{(2\pi)} \frac{e^{iq(j-j')}e^{-i\omega_n(\tau-\tau')}}{\omega_n^2 + \omega(q)^2} \\
&= \frac{a}{2m}\int_{-\pi}^{\pi}\frac{dq}{2\pi}\frac{e^{iq(j-j')}}{\omega(q)}\left[e^{-\omega(q)|\tau-\tau'|} + 2N(\omega(q))\cosh(\omega(q)(\tau'-\tau)) \right],
\end{aligned}
\tag{9}
$$

where $N(\omega(q))$ is the Bose distribution and the phonon dispersion relation is given by $\omega^2(q) = \omega_{\parallel}^2 + \omega_{\perp}^2\sin(q/2)^2$. The action is quadratic in the phonon field and can be easily integrated, rendering the effective action for coupled spin chains

$$S_{eff} = \sum_j S_{spin}[\phi^j] - \frac{g^2}{2}\sum_{j,j'} \int dx \int d\tau\, d\tau' \left(:\cos(\sqrt{2\pi}\phi^j(x,\tau)): G^{jj'}(\tau,\tau') :\cos(\sqrt{2\pi}\phi^{j'}(x,\tau')): \right). \tag{10}$$

We find it convenient to separate the in-chain from the inter-chain interactions writing

$$S_{eff} = \sum_j S_{spin}[\phi^j] + S_{in} + S_{inter} \tag{11}$$

where

$$S_{in} = -\frac{g^2}{2}\sum_j \int dx \int d\tau\, d\tau' \left(:\cos(\sqrt{2\pi}\phi^j(x,\tau)): G^{jj}(\tau,\tau') :\cos(\sqrt{2\pi}\phi^j(x,\tau')): \right) \tag{12}$$

and

$$S_{inter} = -\frac{g^2}{2} \sum_{j \neq j'} \int dx \int d\tau \, d\tau' \left(: \cos(\sqrt{2\pi}\phi^j(x,\tau)) : G^{jj'}(\tau,\tau') : \cos(\sqrt{2\pi}\phi^{j'}(x,\tau')) : \right). \tag{13}$$

We will now treat the inter-chain interaction with a mean field decoupling. Following Delfino *et. al.*[12], we write

$$: \cos(\sqrt{2\pi}\phi^j) := \epsilon_0 + N(\cos(\sqrt{2\pi}\phi^j)), \tag{14}$$

where the normal order N is now taken with respect to the vacuum of the coupled chains system. Here ϵ_0 represents the subtraction of the staggered energy density ($\epsilon_0(x = ia) \sim (-1)^{i+1}(< \vec{S}_i^j \cdot \vec{S}_{i+1}^j > - < \vec{S}_{i+1}^j \cdot \vec{S}_{i+2}^j >)$) in the coupled system, describing the magnetic dimerization along chains. According to the dimerization picture, we take ϵ_0 to be position independent. Then

$$S_{inter} = -\frac{g^2}{2} \sum_{j \neq j'} \int dx \int d\tau \, d\tau' \left\{ \epsilon_0^2 \, G^{jj'}(\tau,\tau') + \epsilon_0 N(\cos(\sqrt{2\pi}\phi^j(x,\tau))) \, G^{jj'}(\tau,\tau') \right.$$

$$\left. + \epsilon_0 N(\cos(\sqrt{2\pi}\phi^{j'}(x,\tau'))) \, G^{jj'}(\tau,\tau') + \cdots \right\} \tag{15}$$

where the ellipsis corresponds to quadratic fluctuations in the inter-chain coupling, which we will neglect at the MF level (*i.e.* we assume that fluctuations are small with respect to the expectation value ϵ_0). Due to isotropy and translation symmetry $G^{jj'}(\tau,\tau') = G^{|j-j'|}(|\tau - \tau'|)$, then the last two terms are equal. Moreover, we can change the summation indices from j, j' to $j, J = j' - j$ and τ, τ' to $\tau, \Theta = \tau' - \tau$ and perform the sum over J and the integral over Θ. We obtain

$$\int_0^\beta d\tau' \sum_{J \neq 0} G^J(|\tau - \tau'|) = \int_0^\beta d\Theta \left(\sum_J G^J(\Theta) - G^0(\Theta) \right)$$

$$= \frac{a}{2m} \{ \frac{1}{\omega_\parallel^2} \left[(1 - e^{-\beta\omega_\parallel}) + 2N(\omega_\parallel) \sinh(\beta\omega_\parallel) \right]$$

$$- \frac{1}{2} \int_{-\pi}^\pi \frac{dq}{2\pi} \frac{1}{\omega(q)^2} \left[(1 - e^{-\beta\omega(q)}) + 2N(\omega(q)) \sinh(\beta\omega(q)) \right] \}, \tag{16}$$

notably leading to the temperature independent result

$$\int_0^\beta d\tau' \sum_{J \neq 0} G^J(|\tau - \tau'|) = \frac{a}{m} \frac{1}{\omega_\parallel^2} \left(1 - \frac{1}{\sqrt{1 + \frac{\omega_\perp^2}{\omega_\parallel^2}}} \right) \equiv F(\omega_\parallel, \omega_\perp). \tag{17}$$

Then, S_{inter} reads

$$S_{inter} = -\epsilon_0^2 \frac{g^2}{2} \sum_j \int dx \, d\tau \, F(\omega_\parallel, \omega_\perp)$$

$$- \epsilon_0 \, g^2 \sum_j \int dx \int d\tau \, N(\cos(\sqrt{2\pi}\phi^j)) \, F(\omega_\parallel, \omega_\perp). \tag{18}$$

After writing the space-time volume integral, and writing back in the last term $N(\cos(\sqrt{2\pi}\phi^j(\tau))) =: \cos(\sqrt{2\pi}\phi^j(\tau)) : -\epsilon_0$, the effective action in eq.(11) takes the mean field form

$$S_{eff}^{\mathcal{MF}} = \sum_j S_{spin}[\phi^j] - \frac{g^2}{2} \sum_j \int dx \, d\tau \, d\tau' : \cos(\sqrt{2\pi}\phi^j(x,\tau)) : G^0(\tau,\tau') : \cos(\sqrt{2\pi}\phi^j(x,\tau')) :$$

$$- \epsilon_0 \, g^2 F(\omega_\parallel, \omega_\perp) \sum_j \int dx \, d\tau \, : \cos(\sqrt{2\pi}\phi^j(x,\tau)) : + \frac{1}{2}\epsilon_0^2 \, g^2 F(\omega_\parallel, \omega_\perp) N L \beta. \tag{19}$$

The second term in the first line is the remaining in-chain retarded interaction. In the antiadabatic limit ($m \to \infty$) it becomes an instantaneous interaction which is a marginally irrelevant perturbation. Following an argument similar as

the one presented in [14] (see the discussion starting from eq.(2.30)), it is possible to show that even in the finite mass case this term gives rise to an irrelevant operator (see also [8]). Consistently with the bosonized spin Hamiltonian in eq.(2), we neglect it in the following.

Finally we obtain

$$S_{eff}^{\mathcal{MF}} = \sum_j S_{spin}[\phi^j] - \epsilon_0\, g^2 F(\omega_\parallel, \omega_\perp) \sum_j \int dx\, d\tau\ : \cos(\sqrt{2\pi}\phi^j(x,\tau)): +\epsilon_0^2 \frac{g^2}{2} F(\omega_\parallel, \omega_\perp) NL\beta. \tag{20}$$

The second term is a strongly relevant perturbation that opens a gap for any value of the phonon frequencies $\omega_\parallel$ and $\omega_\perp$, as long as ϵ_0 does not vanish (this will be evaluated by a self-consistent procedure in the next section). Note that this behavior is different than the one obtained in a pure one-dimensional model[8]. In that case, going from the adiabatic to the antiadiabatic limit, the gap closes at an intermediate value of the phonon frequency. Our previous discussion shows that when the 2 or 3D character of the phonons is taken into account such a crossover does not show up. In [12] a model similar to (1) has been considered only in the antiadiabatic limit; our results show that their fully gapped phase extends over a finite frequency range. In addition, as we have kept the explicit dependence on the phonon frequencies, we can analyze the evolution of the gap and the SP transition temperature. We will undertake this analysis in the following section.

III.   THE SPIN GAP AND TRANSITION TEMPERATURE AS A FUNCTION OF THE PHONON FREQUENCY

Let us start by discussing how the Mean Field adiabatic treatment of the phonon field can be implemented in our calculation. This will give results for the spin gap and the transition temperature generalizing those in [13], which are in fact extensions of the classical work of Cross and Fisher[1]. This calculation will set up the energy and temperature scale to be compared with our more general non-adiabatic results. Fixing the displacement field in eq.(7) to be a constant (chain, position and time independent) $u^j(x,\tau) = u$, we have

$$S_{ad} = N \left[S_{spin}[\phi] - gu \int dx d\tau : \cos(\sqrt{2\pi}\phi(x,\tau)): +\frac{m}{2a}L\beta\omega_\parallel^2 u^2 \right]. \tag{21}$$

Note that the term with $\omega_\perp$ vanishes and therefore the total action is N times the action of each chain.

We obtain u in a self-consistent way by minimizing the total energy with respect to it. The ground state energy is evaluated using the exact results for the massive sine-Gordon theory. The lowest energy excitation is a soliton of mass M_{ad}, which can be obtained from eq. (12) of [7] ($2\mu = gu/v_F$ and $\beta = 1/2$ in our notation):

$$\frac{gu}{2v_F} = \frac{\Gamma(\frac{1}{4})}{\pi\Gamma(\frac{3}{4})} \left[M_{ad}v_F\sqrt{\frac{\pi}{4}\frac{\Gamma(\frac{2}{3})}{\Gamma(\frac{1}{6})}} \right]^{\frac{3}{2}}. \tag{22}$$

The specific ground state energy for the sine-Gordon theory is given by $-\frac{1}{4}M_{ad}^2 v_F^3 \tan(\frac{\pi}{6})$, so that the total energy density reads

$$e^{ad} \equiv \frac{E^{ad}}{NL} = \frac{m}{2a}\omega_\parallel^2 u^2 - \frac{1}{4}M_{ad}^2 v_F^3 \tan(\frac{\pi}{6}). \tag{23}$$

Inverting (22) to obtain $M_{ad}(u)$ and minimizing (23) with respect to u we get:

$$M_{ad} = \frac{g^2}{4v_F^2}\frac{a}{m\omega_\parallel^2}\frac{1}{3}\tan(\frac{\pi}{6})\left(\frac{\pi\Gamma(\frac{3}{4})}{\Gamma(\frac{1}{4})}\right)^2\left(\sqrt{\frac{4}{\pi}\frac{\Gamma(\frac{1}{6})}{\Gamma(\frac{2}{3})}}\right)^3 \equiv H\frac{g^2}{v_F^2}\frac{a}{m\omega_\parallel^2}, \tag{24}$$

where $H = 5.4133$ is just a constant collecting all of the numerical factors. The spin gap Δ^{ad} is then given by

$$\Delta^{ad} = M_{ad}v_F^2. \tag{25}$$

Equations (24) and (25) give the zero temperature gap in terms of the model parameters g, $J_\parallel$ and $\omega_\parallel$. It is equivalent to the first of the eqs. (8) in[13].

In the Mean Field adiabatic treatment, the spin-Peierls transition temperature T_{SP}^{ad} can be obtained by considering the finite temperature free energy. Borrowing the appropriate expansion in powers of u from Eq. (12) of [13] ($\frac{2g\delta}{(2\pi a)^2}$ must be replaced by $gu/\sqrt{a}$) the lowest order of the sine-Gordon model free energy density reads

$$-\frac{\pi}{6v_F}T^2 - \frac{\pi^2}{4\Gamma^4(\frac{3}{4})}\frac{(gu)^2}{T} + O(u^4),\qquad(26)$$

so that the full variational free energy is obtained by adding the contribution of the elastic energy,

$$f^{ad} \equiv \frac{F^{ad}}{NL} = \frac{m}{2a}\omega_{\parallel}^2 u^2 - \frac{\pi}{6v_F}T^2 - \frac{\pi^2}{4\Gamma^4(\frac{3}{4})}\frac{(gu)^2}{T} + O(u^4).\qquad(27)$$

The transition temperature corresponds to the one where the free energy minimum shifts from $u \neq 0$ to $u = 0$. Although we have not written quartic terms in u, it is easy to see that the transition is signaled by a change of sign in the coefficient of u^2. This condition gives

$$T_{SP}^{ad} = \frac{ag^2\pi^2}{2\Gamma^4(\frac{3}{4})m\omega_{\parallel}^2}.\qquad(28)$$

We now undertake the calculation of the gap and the transition temperature in the non adiabatic case. We start from the action (20), our main result previously obtained. Comparing eqs. (20) and (21) we note that the soliton mass M can be computed by following similar steps as we did to obtain M^{ad}. Now, the mean field variational parameter is ϵ_0 instead of u (indeed the factor $gF\epsilon_0$ plays the role of u); the total energy density is given by

$$e \equiv \frac{E}{NL} = \frac{\epsilon_0^2 g^2}{2}F(\omega_{\parallel},\omega_{\perp}) - \frac{1}{4}M^2 v_F^3 \tan(\frac{\pi}{6}).\qquad(29)$$

We readily obtain the soliton mass as

$$M = H\frac{g^2}{v_F^2}F(\omega_{\parallel},\omega_{\perp}),\qquad(30)$$

and the corresponding gap $\Delta = Mv_F^2$. Comparing this result with eq.(24) we obtain the relation between the gap in the non-adiabatic and the adiabatic case:

$$\frac{\Delta}{\Delta_{ad}} = 1 - \frac{1}{\sqrt{1+(\frac{\omega_{\perp}}{\omega_{\parallel}})^2}}.\qquad(31)$$

In Fig. 1 we show the evolution of the gap with the ratio $\frac{\omega_{\perp}}{\omega_{\parallel}}$. Only for $\frac{\omega_{\perp}}{\omega_{\parallel}} \to \infty$, $i.e.$ when the lines perpendicular to the chain move rigidly, the gap corresponds to the adiabatic one. Note that this is precisely the condition established by CF for the validity of their RPA calculations. In the general case the gap decreases when $\frac{\omega_{\perp}}{\omega_{\parallel}}$ decreases. This is an important result applicable to a general non-adiabatic spin-Peierls system. For example, for $CuGeO_3$ we can take as the relevant phonon mode (with frequency $\omega_{\parallel}$) the projections of the (0.5 0 0.5) phonons on the direction of the magnetic chains. The transverse direction is then the b-direction along the path (0.5 x 0.5). The phonon dispersion relation $\omega^2(q) = \omega_{\parallel}^2 + \omega_{\perp}^2 \sin(q/2)^2$ in our model corresponds to phonons in this direction. We estimate $\omega_{\perp}$ from the frequencies at the center and at the boundary of the Brillouin zone in this direction. It has been recognized that there are two T_+^2 phonons at (0.5 0 0.5) which are the relevant for the SP distortion (with frequencies $\omega_1 = 3.12\,THz$ and $\omega_2 = 6.53\,THz$ at room temperature)[4]. From Fig. 12 in [5] we can follow the dispersion of the branches in the direction (0.5 x 0.5) connected with these two modes. The lowest energy branch is rather flat and we do not take it into account. For the phonon with the frequency ω_2 we have $\frac{\omega_{\perp}}{\omega_{\parallel}} \sim 0.58$ and the gap from eq. (31) is reduced to 13% of the one estimated by the adiabatic approximation. In practice, the measured zero temperature gap is used to estimate the spin-phonon coupling[15]. Our previous result implies that the spin-phonon coupling could be strongly underestimated by using adiabatic results. Indeed, from our present approach we estimate the dimensionless spin-phonon coupling ($\lambda = \frac{J\alpha^2}{K}$) for $CuGeO_3$ one order of magnitude larger than the previously calculated one. This could have important consequences to interpret experimental results in this and other materials.

A relation similar to eq. (31) holds between the transition temperature in the non-adiabatic and the adiabatic case. The free energy corresponding to action (20) should be expanded in powers of ϵ_0. We take again this expansion from Eq. (12) of [13] (now $\frac{2g\delta}{(2\pi a)^2}$ is replaced by $\epsilon_0 g^2 F(\omega_{\parallel},\omega_{\perp})/\sqrt{a}$). The total free energy density is

$$f \equiv \frac{F}{NL} = -\frac{\pi}{6v_F}T^2 + \epsilon_0^2\frac{g^2 F(\omega_{\parallel},\omega_{\perp})}{2}\left(1 - \frac{g^2\pi^2 F(\omega_{\parallel},\omega_{\perp})}{2\Gamma^4(\frac{3}{4})T}\right).\qquad(32)$$
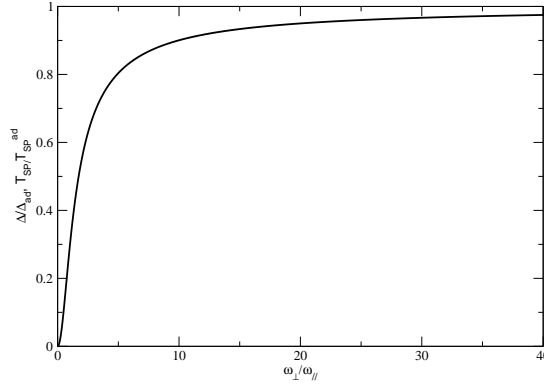
FIG. 1: Dependence of the gap and the SP temperature with $\frac{\omega_\perp}{\omega_\parallel}$.

The vanishing of the factor proportional to ϵ_0^2 signals the transition temperature. We get

$$T_{SP} = \frac{g^2\pi^2}{2\Gamma^4(\frac{3}{4})} F(\omega_\parallel, \omega_\perp) \tag{33}$$

and the promised relation is:

$$\frac{T_{SP}}{T_{SP}^{ad}} = 1 - \frac{1}{\sqrt{1 + (\frac{\omega_\perp}{\omega_\parallel})^2}}. \tag{34}$$

Notice that the ratio $\frac{\Delta}{T_{SP}}$ from our computation does not depend on $\frac{\omega_\perp}{\omega_\parallel}$. The value of such a ratio seems to be fixed by the adiabatic calculation. The existence of such universal ratio is similar to the BCS mean field theory of superconductivity. Moreover, the experimental value observed in $CuGeO_3$ is close to the BCS-ratio 1.76. In fact a BCS-like theory could be obtained from the original Heisenberg model coupled to phonons by a Jordan-Wigner transformation and neglecting interaction between the spinless fermions. Note however that the spinless fermions are strongly interacting, and this fact renormalizes the BCS ratio away from the non interacting value[13]. The precise value of this ratio is difficult to obtain because it is affected by logarithmic corrections induced by marginally irrelevant terms. Indeed, the effect of the marginal term arising from the Heisenberg interaction is expected to be small in $CuGeO_3$ because the second next-nearest neighbor is closer to the critical value[15], where logarithmic corrections vanish. However, as can be seem from action (11), logarithmic corrections are also expected from the spin-phonon interaction term and they do depend on the phonon frequencies. Therefore we expect that the exact value of $\frac{\Delta}{T_{SP}}$ will ultimately depend on $\frac{\omega_\perp}{\omega_\parallel}$.

IV. DYNAMICS OF THE PHONON MODES

The original work of CF on spin-Peierls systems predicts the softening of a phonon mode above the transition temperature, whose polarization pattern corresponds to the static distortion leading to the low temperature phase below the transition point T_{SP}. The softening is due to the coupling of the phonons with the one-dimensional magnetism. This is in fact a quite general scenario for a structural displacive phase transition. Therefore it came as a surprise that the SP transition in $CuGeO_3$ shows no phonon softening[19,20]. Gros and Werner[6] have reanalyzed the CF approach showing that, for higher enough bare phonon frequency, there is a second pole of the phonon propagator without softening of the active SP phonon, characterized by the presence of a central peak in the dynamical structure factor near the transition point. Moreover, the RPA approach underlying the CF calculation is justified if the SP phonon has a bare frequency considerably lower than other momentum phonons, *i.e.* a non-magnetic softening observable at high temperature relative to the SP transition temperature. This is not the situation in $CuGeO_3$ and application of RPA seems questionable.

In the following we show how by extending our previous calculations to the dynamics of the phonon modes we can solve this puzzle. The extension of the static MF approximation on the interchain interaction to the dynamical correlation function is accomplished by a RPA analysis along the lines of [12,21]. In contrast to the one-dimensional

analysis in CF, this RPA is based on the *quasi*-one-dimensionality underlying this kind of materials, and does not require a preexisting mode softening. It becomes exact in the limit of an infinite number of neighboring chains.

The dressed phonon frequencies are obtained from the poles of the retarded phonon Green's function $D(k,q,\omega)$[16] which can be computed from the Matsubara Green's function $D(k,q,\omega_n)$, with wave vectors k in the chain direction and q the transverse one, by analytic continuation as $D(k,q,\omega) = D(k,q,i\omega_n \to \omega)$. This is in fact the Fourier transform of the Green's function in real space and imaginary time $D^{j-j'}(x-x',\tau-\tau')$, which can be found by functional derivation of the partition function when a current term is added:

$$Z[J] = \int \mathcal{D}u^j \mathcal{D}\phi^j \exp\left\{ -\sum_j \int dx\, d\tau [\mathcal{L}(\phi^j(x,\tau), u^j(x,\tau)) + gJ^j(x,\tau)u^j(x,\tau)] \right\}. \tag{35}$$

Integrating out the phonon coordinates as before we obtain the following effective action

$$\begin{aligned} S_{eff} &= \sum_j S_{spin}[\phi^j] \\ &- \frac{g^2}{2} \sum_{j,j'} \int dx \int d\tau d\tau' \left(:\cos(\sqrt{2\pi}\phi^j(x,\tau)): + J^j(x,\tau) \right) G^{jj'}(\tau,\tau') \left(:\cos(\sqrt{2\pi}\phi^{j'}(x,\tau')): + J^{j'}(x,\tau') \right). \end{aligned} \tag{36}$$

The dressed phonon propagator

$$D^{j-j'}(x-x',\tau-\tau') = \frac{1}{g^2} \frac{\delta^2 \ln Z[J]}{\delta J^{j'}(x',\tau')\delta J^j(x,\tau)}\bigg|_{\{J^j(x,\tau)\}=0} \tag{37}$$

can be obtained from eqs. (35, 36, 37) as

$$\begin{aligned} D^{j-j'}(x-x',\tau-\tau') &= G^{j'-j}(x'-x,\tau'-\tau) - g^2 \sum_{\hat{j},\hat{j}'} \int d\hat{x}d\hat{x}'d\hat{\tau}d\hat{\tau}' G^{\hat{j}-j}(\hat{x}-x,\hat{\tau}-\tau)G^{\hat{j}'-j'}(\hat{x}'-x',\hat{\tau}'-\tau') \\ &\qquad \langle \mathcal{T}\left(:\cos(\sqrt{2\pi}\phi^{\hat{j}}(\hat{x},\hat{\tau})):: \cos(\sqrt{2\pi}\phi^{\hat{j}'}(\hat{x}',\hat{\tau}')): \right)\rangle, \end{aligned} \tag{38}$$

where $G^{j-j'}(x-x',\tau-\tau') = \delta(x-x')G^{jj'}(\tau,\tau')$ is a convenient notation for the non-interacting phonon propagator and $\mathcal{T}$ indicates Euclidean time-ordering. After Fourier transforming to (k,q,ω_n) coordinates and performing the analytic continuation $i\omega_n \to \omega$ we obtain the desired retarded phonon Green's function

$$D(k,q,\omega) = G(q,\omega) + g^2 G^2(q,\omega)\chi(k,q,\omega), \tag{39}$$

where $G(q,\omega) = \frac{a}{m}\frac{1}{-\omega^2+\omega(q)}$ is the bare phonon Green's function and $\chi(k,q,\omega)$ stems for the Fourier transform of the retarded correlator of $:\cos(\sqrt{2\pi}\phi^j):$. In order to evaluate bulk corrections arising from inter-chain coupling, we will calculate this correlator using a RPA approach in the interchain interaction[12]. It reads

$$\chi^{RPA}(k,q,\omega) = \frac{\chi^0(k,\omega;T)}{1 - g^2 G_{inter}(q,\omega)\chi^0(k,\omega;T)}, \tag{40}$$

where $\chi^0(k,\omega;T)$ is the already known finite temperature one chain $:\cos(\sqrt{2\pi}\phi):$-correlator and G_{inter} is the inter-chain bare phonon propagator, defined in coordinate space by the subtraction

$$G^{j-j'}_{inter}(x-x',\tau-\tau') = G^{j-j'}(x-x',\tau-\tau') - \delta^{jj'} G^0(x-x',\tau-\tau'). \tag{41}$$

The one chain $:\cos(\sqrt{2\pi}\phi):$-correlator at finite temperature has been computed elsewhere[1,6,18], being given by

$$\chi^0(k,\omega;T) = \frac{2d}{T} I_1\left(\frac{(\omega-\Delta)}{2\pi T}\right) I_1\left(\frac{(\omega+\Delta)}{2\pi T}\right), \tag{42}$$

where $d \sim 0.37$ is a constant weakly depending of the momentum cutoff in the bosonization procedure, $\Delta = v_F|k-\pi|$ is the lower edge of the two spinon continuum, and

$$\begin{aligned} I_1(k) &= \frac{1}{2\pi} \int_0^\infty dx e^{ikx}(\sinh(x))^{-\frac{1}{2}} = \\ &\qquad \frac{1}{2\sqrt{2\pi}} \frac{\Gamma[\frac{1}{4} - i\frac{k}{2}]}{\Gamma[\frac{3}{4} - i\frac{k}{2}]}. \end{aligned} \tag{43}$$

It will be useful to note that at low frequency one can expand

$$T\chi^0(k,\omega;T) \approx \chi_0 - i\chi_1 \frac{\omega}{2\pi T} + \chi_2 \left(\frac{\omega}{2\pi T}\right)^2, \tag{44}$$

with $\chi_0 \sim 0.26$ and $\chi_2 \sim 2.2$.

The Fourier transform of the interchain propagator G^{inter} is obtained (see Section II) as

$$G^{inter}(q,\omega) = \frac{1}{-\omega^2 + \omega(q)} - \Upsilon(\omega), \tag{45}$$

with

$$\Upsilon(\omega) = \frac{1}{2\pi} \int \frac{dq'}{\omega^2(q') - \omega^2} = \frac{1}{\sqrt{(\omega_\parallel^2 - \omega^2)}\sqrt{(\omega_\parallel^2 + \omega_\perp^2 - \omega^2)}}. \tag{46}$$

We are interested in the temperature evolution of the SP active phonon mode, given by $k = \pi$ and $q = 0$. From eq.(39-45) we have

$$D(0,\pi,\omega) = \frac{g^2(1 - g^2\Upsilon(\omega)\chi^0(\pi,\omega;T))}{G^{-1} + \frac{g^2}{2}(1 - G^{-1}\Upsilon(\omega))\chi^0(\pi,\omega;T)} \tag{47}$$

and the phonon frequencies are given by the poles over the real axis of this expression, *i.e.* the roots of the following equation

$$-\omega^2 + \omega_\parallel^2 + \frac{g^2}{2}(1 - (\omega_\parallel^2 - \omega^2)\Upsilon(\omega))Re\chi^0(\pi,\omega;T) = 0. \tag{48}$$

Let us start the analysis of the consequences of the previous results by recalculating the spin-Peierls transition temperature. Note that, different than the previous Section, we are now coming from the high temperature phase to the transition point. As discussed by GW, T_{SP} is signaled by a macroscopic occupation of the Peierls active phonon mode, *i.e.* the transition temperature takes place when eq. (48) has a solution $\omega = 0$. We then obtain

$$T_{SP} = \frac{\chi_0 g^2}{2\omega_\parallel^2} \left(1 - \frac{1}{\sqrt{1 + \frac{\omega_\perp^2}{\omega_\parallel^2}}}\right). \tag{49}$$

It is important to stress that eq. (49) gives the same dependency of T_{SP} on the microscopic parameters than eq. (33) in the previous Section; differences in the numerical prefactor arise from different criteria to fix the momentum cutoff. Note however that relation (34) is fulfilled. This results prove that our RPA procedure contains the previous MF approach when the static properties are considered.

In the rest of this Section we face the question of phonon softening, discussing the calculation of the renormalized phonon frequencies. We use (49) to eliminate the cut-off dependent coupling g^2 from eq. (48). After straightforward algebra we obtain

$$\chi_0 \left(1 - \frac{1}{\sqrt{1 + (\frac{\omega_\perp}{\omega_\parallel})^2}}\right) \left(\left(\frac{\omega}{\omega_\parallel}\right)^2 - 1\right) \bigg/ \left(1 - \frac{\sqrt{1 - (\frac{\omega}{\omega_\parallel})^2}}{\sqrt{1 + (\frac{\omega_\perp}{\omega_\parallel})^2 + (\frac{\omega}{\omega_\parallel})^2}}\right) = T_{SP} Re\chi^0(\pi,\omega). \tag{50}$$

This equation is the generalization of the GW results to finite values of $\frac{\omega_\perp}{\omega_\parallel}$, and agrees with their corresponding eq. (6) when $\frac{\omega_\perp}{\omega_\parallel} \gg 1$. There are two different temperature dependence regimes of the renormalized phonon frequency $\omega(\pi,0)$, as depicted in Fig. 2. For low enough $\omega_\parallel$ the phonon progressively softens from higher T until T_{SP}, where it drops to zero frequency. In this regime the phonon softening explains the SP transition. For higher $\omega_\parallel$, the phonon frequency remains finite up to the SP temperature and no soft phonon behavior is obtained; in fact, there can be partial softening or even hardening of the renormalized frequency close to T_{SP}. However, an additional solution $\omega = 0$ in eq. (50) signals the appearance of a central peak in the dynamical structure factor, leading to the SP transition[6].

The limiting value of $\omega_\parallel/T_{SP}$ for separation of regimes depends on $\omega_\perp$. To find this transition analytically it is enough to compare concavities of both sides of eq. (50) at $T = T_{SP}$, as seen in Fig. 2. Expanding both sides up
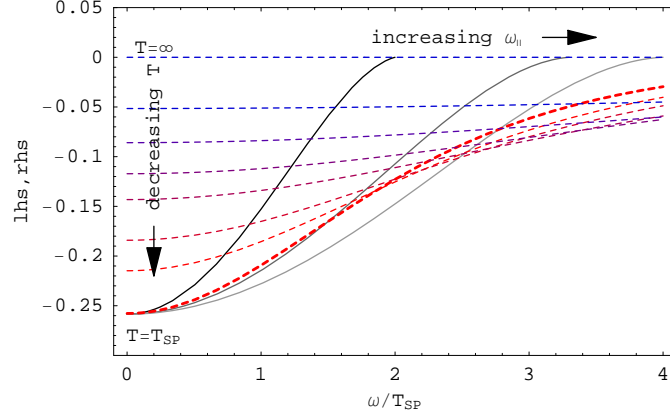
FIG. 2: Evolution of the SP relevant phonon mode. Dashed lines, from blue to red, represent the rhs of eq. (50) when temperature is lowered until T_{SP}. Solid gray lines represent the lhs for $\omega_{\parallel}/T_{SP} = 2, 3, 4$ and $\omega_{\perp}/T_{SP} = 1$. The intersections illustrate the evolution of the renormalized phonon frequency. For $\omega_{\parallel}/T_{SP} = 2$ the phonon softens completely, for $\omega_{\parallel}/T_{SP} = 3$ it softens partially, and for $\omega_{\parallel}/T_{SP} = 4$ it hardens close to T_{SP}.

to second order in $\frac{\omega}{T_{SP}}$, the soft phonon regime is reached when, at $T = T_{SP}$, the coefficient of ω^2 in the r.h.s. is smaller than the one in the l.h.s. Under this condition the bare phonon frequency (that obtained at hight T) evolves continuously to zero when the temperature is lowered until the transition temperature. The following inequality should then be fulfilled to have the soft phonon regime:

$$\frac{\omega_{\parallel}}{T_{SP}} < 2\pi \sqrt{\frac{\chi_0}{\chi_2}} \sqrt{1 + \frac{1}{2} \frac{(1 + \sqrt{1 + (\omega_{\perp}/\omega_{\parallel})^2})}{1 + (\omega_{\perp}/\omega_{\parallel})^2}}. \tag{51}$$

In the other case, the bare phonon frequency evolves to some finite value at the SP transition. In Fig. 3 we show the phase diagram of the spin-phonon system on the $\omega_{\perp} - \omega_{\parallel}$ plane. Note that in a wide range of high enough $\frac{\omega_{\perp}}{T_{SP}}$ the separatrix is given by $\frac{\omega_{\parallel}}{T_{SP}} \sim 2.2$ as in GW. Our result extends this condition for finite values of $\frac{\omega_{\perp}}{T_{SP}}$ where realistic spin-Peierls materials as $CuGeO_3$ live. This also explains why the RPA approach for the spin-phonon coupling underlying the GW calculation compares well with experiments on $CuGeO_3$.

In Fig. 4 we show the temperature dependence of the renormalized phonon frequency for $\frac{\omega_{\perp}}{T_{SP}} = 1$ where the phase diagram of Fig. 3 is not completely flat. The behavior shifts from a soft to a non soft phonon regime at some intermediate value of $\frac{\omega_{\parallel}}{T_{SP}}$. In this last regime the mechanism of the SP transition has been associated with the emergence of a central peak in the spectral signal measured in neutron scatering experiments[22]. For high enough $\frac{\omega_{\parallel}}{T_{SP}}$ the phonon hardens from a minimum value at some intermediate temperature. At $T = T_{SP}$ the frequency of the phonon is the bare one as in the high temperature limit. We will use this fact to fix $\omega_{\parallel}$ for $CuGeO_3$. Note that the T-dependence of the phonon is similar to the one obtained by GW but the frequency and temperature scale are different.

From the previous results we can follow the T-dependence of the Peierls active phonons in $CuGeO_3$. In Fig. 4 (b), we show our prediction for the higher energy mode T_2^+, which is the most anomalous and strongly coupled to the magnetism[4]. We take as a bare phonon frequency $\omega_{\parallel} = 6.8 THz$ i.e. its low temperature value. For $\omega_{\perp}$ we use the relationship obtained in the previous Section. Note that a value of $T_{SP} = 14.1K (0.294 THz)$ has been used to give the frequencies in Thz and the temperatures in K. Our results compare well with Fig. 3 of [4]. In fact we predict a stronger hardening than the one experimentally observed (7% against 4.5% seen in the experiment). This could be due to the simplified model we use, which does not take into account the fact that two phonon modes are necessary to describe the SP transition in $CuGeO_3$[4].

Besides, we can make a prediction for the phonon frequency behavior at higher temperature than the one already measured. It should increase as shown in Fig. 4, approaching the bare frequency at very high T. We note that at room temperature the phonon frequency does not correspond to the bare one as expected. It is almost the minimum of the predicted phonon frequency. The bare frequency is only obtained at $T = T_{SP}$ and at very high temperature (probably not experimentally accessible).

To summarize the results of the present Section, we have generalized the MF approach of the previous Section to the dynamical correlation functions in the high temperature phase. Our approach relies on a RPA on the effective interchain coupling generated by the spin-phonon interaction. In contrast to the previous theoretical calculations,
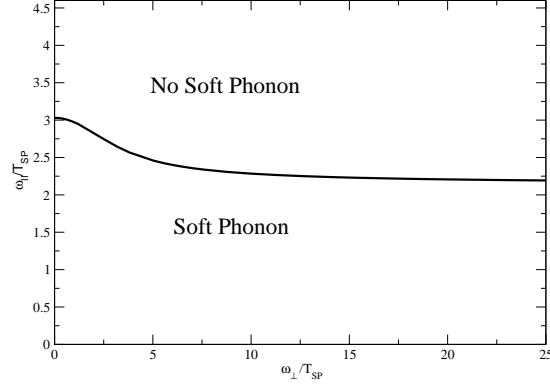
FIG. 3: The line separating the zone in the $\frac{\omega_\perp}{T_{SP}}$, $\frac{\omega_\parallel}{T_{SP}}$ plane, where the spin-Peierls transition takes place by softening of the phonon from the one where the Peierls active phonon does not soften completely.
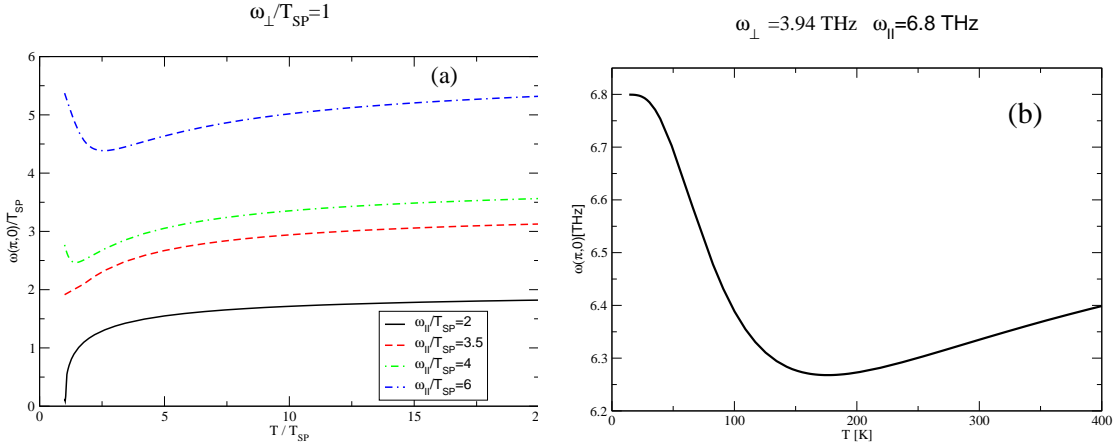

FIG. 4: (a)The temperature dependence of the renormalized phonon frequency for different values of the bare $\frac{\omega_\parallel}{T_{SP}}$, with $\frac{\omega_\perp}{T_{SP}}=1$ (b) The hardening of the phonon for the parameters describing the higher energy active SP mode in CuGeO$_3$. The bare values used for $\omega_\parallel$ and $\omega_\perp$ are shown on top of the Figure.

the present one does not presuppose the existence of a soft phonon mode in the non magnetic regime. Therefore, it can been applied to CuGeO$_3$. Moreover, the qualitative behavior of the Peierls active phonon is similar to the one previously obtained. There is a regime corresponding to low frequency phonon where the structural phase transition takes place by progressive softening of a phonon from the high temperature phase. For higher bare phonon frequency no soft phonon is observed and it can even harden from the room temperature value to the transition temperature one. This is precisely the behavior seen in neutron scattering measurements of the phonon spectra in CuGeO$_3$.

V.   CONCLUSIONS

We have developed a route for the spin-Peierls transition which goes beyond the usual adiabatic treatment of the phonon field. We emphasized the essential character that plays the dispersion of the phonon in the transversal direction to the magnetic chains. Moreover, the results of the present paper show that, when the adiabatic hypothesis for the phonon coordinates is relaxed, the one-chain model does not represent a good starting point to describe a real system. Furthermore the effective interchain interaction generated by the phonons is an essential ingredient for the opening of the gap and the existence of a finite temperature phase transition. The precise determination of the SP transition temperature from the microscopic parameters strongly depends on the width of the transversal phonon dispersion.

Our approach for the dynamics of the phonon mode in the high temperature phase justifies and generalizes previous calculations of the phonon spectra based on the Cross and Fisher early work. Applied to CuGeO$_3$, we show that

the phonon does not soften until the phase transition. Moreover the overall temperature dependence of the phonon frequency is consistent with experimental determinations.

As the elastic interaction between the chains play a central rol in non-adiabatic spin-Peierls systems, we anticipate that a change in the relative positions of the magnetic ions in different chains will change the phase diagram and the mechanism of the phase transition. In this sense it is highly interesting to study the recently discovered quasi-one-dimensional magneto-elastic system TiOCl with an intermediate incommensurate phase where the Ti ions are not aligned in the direction perpendicular to the magnetic chain[3]. We will study in a forthcoming work this system within the formalism developed in the present paper.

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The spin-Peierls transition beyond the adiabatic approximation

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We develop a theory of the spin-Peierls transition taking into account the three dimensional character of the phonon field. Our approach does not rely on the adiabatic or mean field treatment for the phonons. It is instead based in the exact integration of the phonon field, the exact long wavelength solution of the one chain spin problem, and then a mean field approximation for the interchain interaction. We show that the spin gap and the critical temperature are strongly reduced due to the finite frequency effects of the phonon coupling transverse to the magnetic chains. We claim that our results should be applicable to the inorganic spin-Peierls compound $CuGeO_3$. We show that the long standing discussion on absence of a soft mode in this compound can be naturally resolved within our theory.

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I. INTRODUCTION

Quasi-one-dimensional electronic and magnetic materials are fascinating objects which have been intensively studied during the last decades. They show a variety of different phases as the magnetically dimerized, unconventional metal and triplet superconductor phases. It is possible to go from one phase to another by changing the experimentally accessible macroscopic parameters: pressure, temperature and the applied magnetic field. The different phases arise from the competition between the Coulomb repulsion between electrons and their coupling with the lattice degrees of freedom. Whereas the essential physics relies on the one-dimensionality of the electronic dynamics, the stabilization of the different phases depends on the three dimensional character of the system and thus on the interchain interaction. Transitions between the different phases are, in a way, a dimensional crossover from 1D to the three dimensionality of any real material.

Spin-Peierls systems are probably the simplest example of quasi-one-dimensional materials. They show a high temperature phase which can be well modelled by a one dimensional antiferromagnetic Heisenberg chain and a low temperature phase with lattice dimerization and spin singlet ground state. The transition between them arises from the competition between the gain in antiferromagnetic energy and the loss in elastic energy. It is indeed possible due to the three dimensional character of the phonon field. It is therefore very attractive to carefully understand the precise character of this transition as a representative of a large class of quasi-one-dimensional materials.

The theory of spin-Peierls (SP) transition was developed in the 1970's in connection with organic quasi-one-dimensional materials. The seminal work of Cross and Fisher[1] (CF) is nowadays taken as the canonical theory of the spin-Peierls transitions. It is based on a RPA approximation for the phonon field, which corresponds to neglecting the dynamics of the phonons. Otherwise the low energy spin correlations are exactly taken into account by the bosonization method. The CF theory is expected to work when the phonon frequency is much smaller than the spin gap. Moreover, CF have shown that corrections to RPA are small if the bare phonon frequency in the direction of the magnetic chain is much smaller than the phonon frequency perpendicular to the chains, that is to say if there is a *preexisting soft mode* before coupling phonons with the magnetism.

In this context the discovery of the first inorganic SP compound $CuGeO_3$ opened the possibility to experimentally study the dimerized phase and the phase transition with unprecedented precision[2]. The recent characterization of a new family of spin-Peierls materials with an incommensurate intermediate phase has renewed the interest on a precise description of the phase transition[3]. The picture that emerges from neutron scattering measurement of the phonon spectra in $CuGeO_3$ is the following[4,5]: at room temperature, there are two phonon modes relevant for the SP transition with $\omega_1 = 3.12\,THz$ and $\omega_2 = 6.53\,THz$ at the (0.5 0 0.5) point of the Brillouin zone. The phonon dispersion transverse to the propagation vectors of these relevant phonons is rather flat[5]. Therefore, *no preexisting soft* mode is observed and the RPA is not a priori justified. Moreover, on lowering the temperature, ω_1 and ω_2 do

not soften at the SP transition, as expected in the CF scenario. This is a strange behavior for a displacive structural phase transition.

On the other hand, Gros and Werner[6] (GW) have identified a parameter regime where the CF approach does not predict a softening of the relevant phonons but instead the appearance of a central peak in the dynamical structure factor at the transition point. The temperature dependence of the Peierls active phonon modes predicted by this analysis are in agreement with neutron scattering determinations in $CuGeO_3$. However the applicability of the adiabatic approximation or RPA in this material is not a priori justified.

In fact, what is missing for a complete understanding of the spin-Peierls transition in $CuGeO_3$, and possibly in other inorganic quasi-one-dimensional materials, is a theory which does not rely on the static approximation for the phonons. A first step in this direction was presented in [12], where the dynamics of the transverse phonons in the antiadiadatic limit was taken into account and the relevance the three dimensional character of the phonons was first brought to light. We give some more elements of such a theory in the present work.

The plan of the paper is as follows. In Section II, we start from a one-dimensional magnetic model coupled to two dimensional phonons and integrate out the phonon coordinates. Then we treat the effective in-chain interaction exactly by bosonization, and the inter-chain interaction by a mean field approximation. In Section III exact results for the 1D sine-Gordon model[7] are used to solve the mean field equations. By comparing with the adiabatic approximation we identify the relevant parameter to analyze the deviations from the adiabatic limit, namely the ratio between the frequency of phonon relevant for the SP transition ($\omega_\parallel$) and the frequency of the phonons transverse to the magnetic chain ($\omega_\perp$). The adiabatic limit is obtained only for high enough value of $\frac{\omega_\perp}{\omega_\parallel}$. Reducing this parameter both the gap and the spin-Peierls temperature are reduced. For $\omega_\perp \to 0$, *i.e.* the pure one dimensional problem, the gap and the SP temperature vanish. We discuss our results in connection with a recent study of the AF chain coupled to one-dimensional phonons[8]. In Section IV we study the dynamics of the SP relevant phonon mode in the high temperature phase, using a RPA on the effective interchain coupling generated by the spin-phonon interaction. We then address the question of absence of softening close to the SP transition. Finally, in Section V we present our conclusions and prospects for future related work.

II. THE EFFECTIVE INTERACTIONS INDUCED BY PHONONS

Let us start by considering a two dimensional system of spin $S = 1/2$ antiferromagnetic Heisenberg chains, with exchange constant $J_\parallel$ along one of the axes of a non-deformed square elastic lattice. We label by j chains, and by i the sites on each chain. The spin-phonon Hamiltonian is given by[9]:

$$H = \sum_{i,j} \frac{(P_i^j)^2}{2m} + \frac{1}{2} K_\parallel \sum_{i,j} (u_{i+1}^j - u_i^j)^2 + \frac{1}{2} K_\perp \sum_{i,j} \left((u_i^{j+1} - u_i^j)^2 \right) + J_\parallel \sum_{i,j} \left(1 + \alpha(u_{i+1}^j - u_i^j) \right) \vec{S}_i^j \cdot \vec{S}_{i+1}^j, \quad (1)$$

where u_i^j are the relevant (scalar) coordinates for ion displacements with respect to equilibrium positions, P_i^j are their conjugate momenta, $K_\parallel$ and $K_\perp$ are the elastic couplings along in-chain and inter-chain ions, respectively, and α measures the deformation effect on the magnetic exchange constants.

In the absence of phonons, we can write the bosonized low energy (long distance along the chains) Hamiltonian for the Heisenberg spin chains[10] as

$$H_{spin}^j = J_\parallel \sum_{i,j} \vec{S}_i^j \cdot \vec{S}_{i+1}^j \sim \frac{v_F}{2} \int dx \left(K_L \left(\partial_x \tilde{\phi}^j(x) \right)^2 + \frac{1}{K_L} \left(\partial_x \phi^j(x) \right)^2 \right), \quad (2)$$

where $x = ia$ (a being the lattice spacing), $\tilde{\phi}^j$ are the fields dual to the scalar fields ϕ^j, defined in terms of their canonical momentum as $\partial_x \tilde{\phi}^j = \Pi^j$, and : : stands for normal order with respect to the isolated chains ground state. The Fermi velocity of left and right excitations and the usual Luttinger parameter K_L depend on the XXZ anisotropy parameter, taking the values $v_F = \frac{\pi}{2} J_\parallel a$ and $K_L = 1$ for the isotropic Heisenberg chain with only nearest neighbor interaction. A marginal term $\lambda : \cos(2\sqrt{2\pi}\phi(x)) :$ has been discarded in eq.(2).

The term coupling spins with phonons can be treated perturbatively by using the continuum expression for the spin energy density

$$\vec{S}_i^j \cdot \vec{S}_{i+1}^j \sim \rho^j(x) = \frac{1}{\sqrt{2\pi}} \partial_x \phi^j(x) + (-1)^i \beta : \cos(\sqrt{2\pi}\phi^j(x)) : + \cdots \quad (3)$$

where β is a non-universal constant and the ellipses indicate higher harmonics[11]. Notice that $: \cos(\sqrt{2\pi}\phi^j) :$ is a relevant operator of scaling dimension $D = 1/2$.

We will also assume that each chain dimerizes in such a way that the distortions can be approximately described as $u_i^j \approx (-1)^i u^j(x)$. Notice however that neighboring chains are not correlated *a priori*. Then

$$u_{i+1}^j - u_i^j \approx (-1)^{i+1}(2u^j(x) + a\partial_x u^j(x)). \tag{4}$$

We will keep only the leading order in the gradient expansion. The interaction Hamiltonian, in the continuum limit and up to leading order in the lattice spacing, then reads

$$H_{int} = \alpha J_\parallel \sum_{i,j}(u_{i+1}^j - u_i^j)\,\vec{S}_i^j \cdot \vec{S}_{i+1}^j = -g\sum_j \int dx\, u^j(x)\, :\cos(\sqrt{2\pi}\phi^j(x)):\,, \tag{5}$$

where $g \sim \frac{2\alpha J_\parallel \beta}{a}$.

Regarding the phonon Hamiltonian, we find it convenient to first construct the corresponding Lagrangian. Up to leading order in the lattice spacing the phonon Lagrangian can be written in the continuum limit as

$$L_{ph} = \frac{m}{2a}\sum_j \int dx \left[(\partial_t u^j(x,t))^2 - (\omega_\parallel^2 + \frac{1}{2}\omega_\perp^2)(u^j(x,t))^2 + \frac{1}{2}\omega_\perp^2 u^j(x,t)u^{j+1}(x,t)\right], \tag{6}$$

where $\omega_\parallel^2 = 4\frac{K_\parallel}{m}$ and $\omega_\perp^2 = 4\frac{K_\perp}{m}$.

Now we can write the action for the complete system and perform the usual Wick rotation $\tau = it$, arriving to the Euclidean action describing the low energy physics at finite temperature T:

$$
\begin{aligned}
S_E = {} & \sum_j S_{spin}[\phi^j] \\
& + \frac{m}{2a}\sum_j \int dx\, d\tau \left((\partial_\tau u^j(x,\tau))^2 + (\omega_\parallel^2 + \frac{1}{2}\omega_\perp^2)(u^j(x,\tau))^2 - \frac{1}{2}\omega_\perp^2 u^{j+1}(x,\tau)u^j(x,\tau)\right) \\
& - g\sum_j \int dx\, d\tau\, u^j(x,\tau)\, :\cos(\sqrt{2\pi}\phi^j(x,\tau)):\,,
\end{aligned} \tag{7}
$$

where j runs from 1 to N, x from 0 to L, τ from 0 to $\beta = 1/T$, and the spin Euclidean action reads

$$S_{spin}[\phi^j] = \frac{1}{2}\int dx\, d\tau \left(\frac{1}{v_F}(\partial_\tau \phi^j(x,\tau))^2 + v_F(\partial_x \phi^j(x,\tau))^2\right). \tag{8}$$

After Fourier transforming $j \to q$ (the wave vector perpendicular to the magnetic chains) , $\tau \to \omega_n$, with $\omega_n = \frac{2\pi n}{\beta}$ the Matsubara frequency, the phonon Green's function reads:

$$
\begin{aligned}
G^{jj'}(\tau,\tau') = {} & \frac{a}{m}\frac{1}{\beta}\sum_n \int_{-\pi}^{\pi}\frac{dq}{(2\pi)}\frac{e^{iq(j-j')}e^{-i\omega_n(\tau-\tau')}}{\omega_n^2 + \omega(q)^2} \\
= {} & \frac{a}{2m}\int_{-\pi}^{\pi}\frac{dq}{2\pi}\frac{e^{iq(j-j')}}{\omega(q)}\left[e^{-\omega(q)|\tau-\tau'|} + 2N(\omega(q))\cosh(\omega(q)(\tau'-\tau))\right],
\end{aligned} \tag{9}
$$

where $N(\omega(q))$ is the Bose distribution and the phonon dispersion relation is given by $\omega^2(q) = \omega_\parallel^2 + \omega_\perp^2 \sin(q/2)^2$. The action is quadratic in the phonon field and can be easily integrated, rendering the effective action for coupled spin chains

$$S_{eff} = \sum_j S_{spin}[\phi^j] - \frac{g^2}{2}\sum_{j,j'}\int dx \int d\tau\, d\tau' \left(:\cos(\sqrt{2\pi}\phi^j(x,\tau)): G^{jj'}(\tau,\tau') :\cos(\sqrt{2\pi}\phi^{j'}(x,\tau')):\right). \tag{10}$$

We find it convenient to separate the in-chain from the inter-chain interactions writing

$$S_{eff} = \sum_j S_{spin}[\phi^j] + S_{in} + S_{inter} \tag{11}$$

where

$$S_{in} = -\frac{g^2}{2}\sum_j \int dx \int d\tau\, d\tau' \left(:\cos(\sqrt{2\pi}\phi^j(x,\tau)): G^{jj}(\tau,\tau') :\cos(\sqrt{2\pi}\phi^j(x,\tau')):\right) \tag{12}$$

and

$$S_{inter} = -\frac{g^2}{2} \sum_{j \neq j'} \int dx \int d\tau \; d\tau' \left(: \cos(\sqrt{2\pi}\phi^j(x,\tau)) : G^{jj'}(\tau,\tau') : \cos(\sqrt{2\pi}\phi^{j'}(x,\tau')) : \right). \tag{13}$$

We will now treat the inter-chain interaction with a mean field decoupling. Following Delfino *et. al.*[12], we write

$$: \cos(\sqrt{2\pi}\phi^j) := \epsilon_0 + N(\cos(\sqrt{2\pi}\phi^j)), \tag{14}$$

where the normal order N is now taken with respect to the vacuum of the coupled chains system. Here ϵ_0 represents the subtraction of the staggered energy density ($\epsilon_0(x = ia) \sim (-1)^{i+1}(< \vec{S}_i^j \cdot \vec{S}_{i+1}^j > - < \vec{S}_{i+1}^j \cdot \vec{S}_{i+2}^j >)$) in the coupled system, describing the magnetic dimerization along chains. According to the dimerization picture, we take ϵ_0 to be position independent. Then

$$S_{inter} = -\frac{g^2}{2} \sum_{j \neq j'} \int dx \int d\tau \; d\tau' \left\{ \epsilon_0^2 \, G^{jj'}(\tau,\tau') + \epsilon_0 N(\cos(\sqrt{2\pi}\phi^j(x,\tau))) \, G^{jj'}(\tau,\tau') \right.$$

$$\left. + \; \epsilon_0 N(\cos(\sqrt{2\pi}\phi^{j'}(x,\tau'))) \, G^{jj'}(\tau,\tau') + \cdots \right\} \tag{15}$$

where the ellipsis corresponds to quadratic fluctuations in the inter-chain coupling, which we will neglect at the MF level (*i.e.* we assume that fluctuations are small with respect to the expectation value ϵ_0). Due to isotropy and translation symmetry $G^{jj'}(\tau,\tau') = G^{|j-j'|}(|\tau - \tau'|)$, then the last two terms are equal. Moreover, we can change the summation indices from j, j' to $j, J = j' - j$ and τ, τ' to $\tau, \Theta = \tau' - \tau$ and perform the sum over J and the integral over Θ. We obtain

$$\int_0^\beta d\tau' \sum_{J \neq 0} G^J(|\tau - \tau'|) = \int_0^\beta d\Theta \left(\sum_J G^J(\Theta) - G^0(\Theta) \right)$$

$$= \frac{a}{2m} \{ \frac{1}{\omega_\parallel^2} \left[(1 - e^{-\beta\omega_\parallel}) + 2N(\omega_\parallel)\sinh(\beta\omega_\parallel) \right]$$

$$- \frac{1}{2} \int_{-\pi}^\pi \frac{dq}{2\pi} \frac{1}{\omega(q)^2} \left[(1 - e^{-\beta\omega(q)}) + 2N(\omega(q))\sinh(\beta\omega(q)) \right] \}, \tag{16}$$

notably leading to the temperature independent result

$$\int_0^\beta d\tau' \sum_{J \neq 0} G^J(|\tau - \tau'|) = \frac{a}{m} \frac{1}{\omega_\parallel^2} \left(1 - \frac{1}{\sqrt{1 + \frac{\omega_\perp^2}{\omega_\parallel^2}}} \right) \equiv F(\omega_\parallel, \omega_\perp). \tag{17}$$

Then, S_{inter} reads

$$S_{inter} = -\epsilon_0^2 \frac{g^2}{2} \sum_j \int dx \; d\tau \; F(\omega_\parallel, \omega_\perp)$$

$$- \epsilon_0 \, g^2 \sum_j \int dx \int d\tau \; N(\cos(\sqrt{2\pi}\phi^j)) \; F(\omega_\parallel, \omega_\perp). \tag{18}$$

After writing the space-time volume integral, and writing back in the last term $N(\cos(\sqrt{2\pi}\phi^j(\tau))) =: \cos(\sqrt{2\pi}\phi^j(\tau)) : -\epsilon_0$, the effective action in eq.(11) takes the mean field form

$$S_{eff}^{\mathcal{MF}} = \sum_j S_{spin}[\phi^j] - \frac{g^2}{2} \sum_j \int dx \; d\tau \; d\tau' : \cos(\sqrt{2\pi}\phi^j(x,\tau)) : G^0(\tau,\tau') : \cos(\sqrt{2\pi}\phi^j(x,\tau')) :$$

$$- \epsilon_0 \, g^2 F(\omega_\parallel, \omega_\perp) \sum_j \int dx \; d\tau \; : \cos(\sqrt{2\pi}\phi^j(x,\tau)) : + \frac{1}{2}\epsilon_0^2 \, g^2 F(\omega_\parallel, \omega_\perp) N L \beta. \tag{19}$$

The second term in the first line is the remaining in-chain retarded interaction. In the antiadabatic limit ($m \to \infty$) it becomes an instantaneous interaction which is a marginally irrelevant perturbation. Following an argument similar as

the one presented in [14] (see the discussion starting from eq.(2.30)), it is possible to show that even in the finite mass case this term gives rise to an irrelevant operator (see also [8]). Consistently with the bosonized spin Hamiltonian in eq.(2), we neglect it in the following.

Finally we obtain

$$S_{eff}^{\mathcal{MF}} = \sum_j S_{spin}[\phi^j] - \epsilon_0\, g^2 F(\omega_\parallel, \omega_\perp) \sum_j \int dx\; d\tau\; : \cos(\sqrt{2\pi}\phi^j(x,\tau)) : + \epsilon_0^2 \frac{g^2}{2} F(\omega_\parallel, \omega_\perp) NL\beta. \tag{20}$$

The second term is a strongly relevant perturbation that opens a gap for any value of the phonon frequencies $\omega_\parallel$ and $\omega_\perp$, as long as ϵ_0 does not vanish (this will be evaluated by a self-consistent procedure in the next section). Note that this behavior is different than the one obtained in a pure one-dimensional model[8]. In that case, going from the adiabatic to the antiadiabatic limit, the gap closes at an intermediate value of the phonon frequency. Our previous discussion shows that when the 2 or 3D character of the phonons is taken into account such a crossover does not show up. In [12] a model similar to (1) has been considered only in the antiadiabatic limit; our results show that their fully gapped phase extends over a finite frequency range. In addition, as we have kept the explicit dependence on the phonon frequencies, we can analyze the evolution of the gap and the SP transition temperature. We will undertake this analysis in the following section.

III.   THE SPIN GAP AND TRANSITION TEMPERATURE AS A FUNCTION OF THE PHONON FREQUENCY

Let us start by discussing how the Mean Field adiabatic treatment of the phonon field can be implemented in our calculation. This will give results for the spin gap and the transition temperature generalizing those in [13], which are in fact extensions of the classical work of Cross and Fisher[1]. This calculation will set up the energy and temperature scale to be compared with our more general non-adiabatic results. Fixing the displacement field in eq.(7) to be a constant (chain, position and time independent) $u^j(x,\tau) = u$, we have

$$S_{ad} = N\left[S_{spin}[\phi] - gu \int dxd\tau : \cos(\sqrt{2\pi}\phi(x,\tau)) : + \frac{m}{2a}L\beta\omega_\parallel^2 u^2\right]. \tag{21}$$

Note that the term with $\omega_\perp$ vanishes and therefore the total action is N times the action of each chain.

We obtain u in a self-consistent way by minimizing the total energy with respect to it. The ground state energy is evaluated using the exact results for the massive sine-Gordon theory. The lowest energy excitation is a soliton of mass M_{ad}, which can be obtained from eq. (12) of [7] ($2\mu = gu/v_F$ and $\beta = 1/2$ in our notation):

$$\frac{gu}{2v_F} = \frac{\Gamma(\frac{1}{4})}{\pi\Gamma(\frac{3}{4})}\left[M_{ad}v_F\sqrt{\frac{\pi}{4}\frac{\Gamma(\frac{2}{3})}{\Gamma(\frac{1}{6})}}\right]^{\frac{3}{2}}. \tag{22}$$

The specific ground state energy for the sine-Gordon theory is given by $-\frac{1}{4}M_{ad}^2 v_F^3 \tan(\frac{\pi}{6})$, so that the total energy density reads

$$e^{ad} \equiv \frac{E^{ad}}{NL} = \frac{m}{2a}\omega_\parallel^2 u^2 - \frac{1}{4}M_{ad}^2 v_F^3 \tan(\frac{\pi}{6}). \tag{23}$$

Inverting (22) to obtain $M_{ad}(u)$ and minimizing (23) with respect to u we get:

$$M_{ad} = \frac{g^2}{4v_F^2}\frac{a}{m\omega_\parallel^2}\frac{1}{3}\tan(\frac{\pi}{6})\left(\frac{\pi\Gamma(\frac{3}{4})}{\Gamma(\frac{1}{4})}\right)^2\left(\sqrt{\frac{4}{\pi}\frac{\Gamma(\frac{1}{6})}{\Gamma(\frac{2}{3})}}\right)^3 \equiv H\frac{g^2}{v_F^2}\frac{a}{m\omega_\parallel^2}, \tag{24}$$

where $H = 5.4133$ is just a constant collecting all of the numerical factors. The spin gap Δ^{ad} is then given by

$$\Delta^{ad} = M_{ad}v_F^2. \tag{25}$$

Equations (24) and (25) give the zero temperature gap in terms of the model parameters g, $J_\parallel$ and $\omega_\parallel$. It is equivalent to the first of the eqs. (8) in[13].

In the Mean Field adiabatic treatment, the spin-Peierls transition temperature T_{SP}^{ad} can be obtained by considering the finite temperature free energy. Borrowing the appropriate expansion in powers of u from Eq. (12) of [13] ($\frac{2g\delta}{(2\pi a)^2}$ must be replaced by $gu/\sqrt{a}$) the lowest order of the sine-Gordon model free energy density reads

$$-\frac{\pi}{6v_F}T^2 - \frac{\pi^2}{4\Gamma^4(\frac{3}{4})}\frac{(gu)^2}{T} + O(u^4),\tag{26}$$

so that the full variational free energy is obtained by adding the contribution of the elastic energy,

$$f^{ad} \equiv \frac{F^{ad}}{NL} = \frac{m}{2a}\omega_\parallel^2 u^2 - \frac{\pi}{6v_F}T^2 - \frac{\pi^2}{4\Gamma^4(\frac{3}{4})}\frac{(gu)^2}{T} + O(u^4).\tag{27}$$

The transition temperature corresponds to the one where the free energy minimum shifts from $u \neq 0$ to $u = 0$. Although we have not written quartic terms in u, it is easy to see that the transition is signaled by a change of sign in the coefficient of u^2. This condition gives

$$T_{SP}^{ad} = \frac{ag^2\pi^2}{2\Gamma^4(\frac{3}{4})m\omega_\parallel^2}.\tag{28}$$

We now undertake the calculation of the gap and the transition temperature in the non adiabatic case. We start from the action (20), our main result previously obtained. Comparing eqs. (20) and (21) we note that the soliton mass M can be computed by following similar steps as we did to obtain M^{ad}. Now, the mean field variational parameter is ϵ_0 instead of u (indeed the factor $gF\epsilon_0$ plays the role of u); the total energy density is given by

$$e \equiv \frac{E}{NL} = \frac{\epsilon_0^2 g^2}{2}F(\omega_\parallel, \omega_\perp) - \frac{1}{4}M^2 v_F^3 \tan(\frac{\pi}{6}).\tag{29}$$

We readily obtain the soliton mass as

$$M = H\frac{g^2}{v_F^2}F(\omega_\parallel, \omega_\perp),\tag{30}$$

and the corresponding gap $\Delta = Mv_F^2$. Comparing this result with eq.(24) we obtain the relation between the gap in the non-adiabatic and the adiabatic case:

$$\frac{\Delta}{\Delta_{ad}} = 1 - \frac{1}{\sqrt{1 + (\frac{\omega_\perp}{\omega_\parallel})^2}}.\tag{31}$$

In Fig. 1 we show the evolution of the gap with the ratio $\frac{\omega_\perp}{\omega_\parallel}$. Only for $\frac{\omega_\perp}{\omega_\parallel} \to \infty$, *i.e.* when the lines perpendicular to the chain move rigidly, the gap corresponds to the adiabatic one. Note that this is precisely the condition established by CF for the validity of their RPA calculations. In the general case the gap decreases when $\frac{\omega_\perp}{\omega_\parallel}$ decreases. This is an important result applicable to a general non-adiabatic spin-Peierls system. For example, for CuGeO$_3$ we can take as the relevant phonon mode (with frequency $\omega_\parallel$) the projections of the (0.5 0 0.5) phonons on the direction of the magnetic chains. The transverse direction is then the b-direction along the path (0.5 x 0.5). The phonon dispersion relation $\omega^2(q) = \omega_\parallel^2 + \omega_\perp^2 \sin(q/2)^2$ in our model corresponds to phonons in this direction. We estimate $\omega_\perp$ from the frequencies at the center and at the boundary of the Brillouin zone in this direction. It has been recognized that there are two T_+^2 phonons at (0.5 0 0.5) which are the relevant for the SP distortion (with frequencies $\omega_1 = 3.12\,THz$ and $\omega_2 = 6.53\,THz$ at room temperature)[4]. From Fig. 12 in [5] we can follow the dispersion of the branches in the direction (0.5 x 0.5) connected with these two modes. The lowest energy branch is rather flat and we do not take it into account. For the phonon with the frequency ω_2 we have $\frac{\omega_\perp}{\omega_\parallel} \sim 0.58$ and the gap from eq. (31) is reduced to 13% of the one estimated by the adiabatic approximation. In practice, the measured zero temperature gap is used to estimate the spin-phonon coupling[15]. Our previous result implies that the spin-phonon coupling could be strongly underestimated by using adiabatic results. Indeed, from our present approach we estimate the dimensionless spin-phonon coupling ($\lambda = \frac{J\alpha^2}{K}$) for CuGeO$_3$ one order of magnitude larger than the previously calculated one. This could have important consequences to interpret experimental results in this and other materials.

A relation similar to eq. (31) holds between the transition temperature in the non-adiabatic and the adiabatic case. The free energy corresponding to action (20) should be expanded in powers of ϵ_0. We take again this expansion from Eq. (12) of [13] (now $\frac{2g\delta}{(2\pi a)^2}$ is replaced by $\epsilon_0 g^2 F(\omega_\parallel, \omega_\perp)/\sqrt{a}$). The total free energy density is

$$f \equiv \frac{F}{NL} = -\frac{\pi}{6v_F}T^2 + \epsilon_0^2\frac{g^2 F(\omega_\parallel, \omega_\perp)}{2}\left(1 - \frac{g^2\pi^2 F(\omega_\parallel, \omega_\perp)}{2\Gamma^4(\frac{3}{4})T}\right).\tag{32}$$
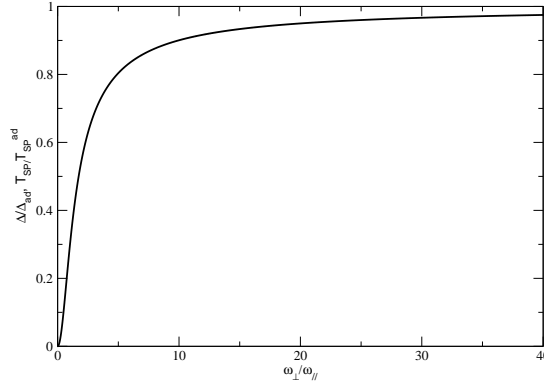
FIG. 1: Dependence of the gap and the SP temperature with $\frac{\omega_\perp}{\omega_\parallel}$.

The vanishing of the factor proportional to ϵ_0^2 signals the transition temperature. We get

$$T_{SP} = \frac{g^2\pi^2}{2\Gamma^4(\frac{3}{4})} F(\omega_\parallel, \omega_\perp) \tag{33}$$

and the promised relation is:

$$\frac{T_{SP}}{T_{SP}^{ad}} = 1 - \frac{1}{\sqrt{1 + (\frac{\omega_\perp}{\omega_\parallel})^2}}. \tag{34}$$

Notice that the ratio $\frac{\Delta}{T_{SP}}$ from our computation does not depend on $\frac{\omega_\perp}{\omega_\parallel}$. The value of such a ratio seems to be fixed by the adiabatic calculation. The existence of such universal ratio is similar to the BCS mean field theory of superconductivity. Moreover, the experimental value observed in $CuGeO_3$ is close to the BCS-ratio 1.76. In fact a BCS-like theory could be obtained from the original Heisenberg model coupled to phonons by a Jordan-Wigner transformation and neglecting interaction between the spinless fermions. Note however that the spinless fermions are strongly interacting, and this fact renormalizes the BCS ratio away from the non interacting value[13]. The precise value of this ratio is difficult to obtain because it is affected by logarithmic corrections induced by marginally irrelevant terms. Indeed, the effect of the marginal term arising from the Heisenberg interaction is expected to be small in $CuGeO_3$ because the second next-nearest neighbor is closer to the critical value[15], where logarithmic corrections vanish. However, as can be seem from action (11), logarithmic corrections are also expected from the spin-phonon interaction term and they do depend on the phonon frequencies. Therefore we expect that the exact value of $\frac{\Delta}{T_{SP}}$ will ultimately depend on $\frac{\omega_\perp}{\omega_\parallel}$.

IV. DYNAMICS OF THE PHONON MODES

The original work of CF on spin-Peierls systems predicts the softening of a phonon mode above the transition temperature, whose polarization pattern corresponds to the static distortion leading to the low temperature phase below the transition point T_{SP}. The softening is due to the coupling of the phonons with the one-dimensional magnetism. This is in fact a quite general scenario for a structural displacive phase transition. Therefore it came as a surprise that the SP transition in $CuGeO_3$ shows no phonon softening[19,20]. Gros and Werner[6] have reanalyzed the CF approach showing that, for higher enough bare phonon frequency, there is a second pole of the phonon propagator without softening of the active SP phonon, characterized by the presence of a central peak in the dynamical structure factor near the transition point. Moreover, the RPA approach underlying the CF calculation is justified if the SP phonon has a bare frequency considerably lower than other momentum phonons, *i.e.* a non-magnetic softening observable at high temperature relative to the SP transition temperature. This is not the situation in $CuGeO_3$ and application of RPA seems questionable.

In the following we show how by extending our previous calculations to the dynamics of the phonon modes we can solve this puzzle. The extension of the static MF approximation on the interchain interaction to the dynamical correlation function is accomplished by a RPA analysis along the lines of [12,21]. In contrast to the one-dimensional

analysis in CF, this RPA is based on the *quasi*-one-dimensionality underlying this kind of materials, and does not require a preexisting mode softening. It becomes exact in the limit of an infinite number of neighboring chains.

The dressed phonon frequencies are obtained from the poles of the retarded phonon Green's function $D(k, q, \omega)^{16}$ which can be computed from the Matsubara Green's function $D(k, q, \omega_n)$, with wave vectors k in the chain direction and q the transverse one, by analytic continuation as $D(k, q, \omega) = D(k, q, i\omega_n \to \omega)$. This is in fact the Fourier transform of the Green's function in real space and imaginary time $D^{j-j'}(x - x', \tau - \tau')$, which can be found by functional derivation of the partition function when a current term is added:

$$Z[J] = \int \mathcal{D}u^j \mathcal{D}\phi^j \exp\left\{ -\sum_j \int dx\, d\tau [\mathcal{L}(\phi^j(x, \tau), u^j(x, \tau)) + gJ^j(x, \tau)u^j(x, \tau)] \right\}. \tag{35}$$

Integrating out the phonon coordinates as before we obtain the following effective action

$$S_{eff} = \sum_j S_{spin}[\phi^j]$$
$$- \frac{g^2}{2} \sum_{j,j'} \int dx \int d\tau d\tau' \left(: \cos(\sqrt{2\pi}\phi^j(x, \tau)) : + J^j(x, \tau)\right) G^{jj'}(\tau, \tau') \left(: \cos(\sqrt{2\pi}\phi^{j'}(x, \tau')) : + J^{j'}(x, \tau')\right). \tag{36}$$

The dressed phonon propagator

$$D^{j-j'}(x - x', \tau - \tau') = \frac{1}{g^2} \frac{\delta^2 \ln Z[J]}{\delta J^{j'}(x', \tau')\delta J^j(x, \tau)}\bigg|_{\{J^j(x,\tau)\}=0} \tag{37}$$

can be obtained from eqs. (35, 36, 37) as

$$D^{j-j'}(x - x', \tau - \tau') = G^{j'-j}(x' - x, \tau' - \tau) - g^2 \sum_{\hat{j},\hat{j}'} \int d\hat{x}d\hat{x}'d\hat{\tau}d\hat{\tau}' G^{\hat{j}-j}(\hat{x} - x, \hat{\tau} - \tau)G^{\hat{j}'-j'}(\hat{x}' - x', \hat{\tau}' - \tau')$$
$$\langle \mathcal{T}\left(: \cos(\sqrt{2\pi}\phi^{\hat{j}}(\hat{x}, \hat{\tau})) :: \cos(\sqrt{2\pi}\phi^{\hat{j}'}(\hat{x}', \hat{\tau}')) :\right)\rangle, \tag{38}$$

where $G^{j-j'}(x - x', \tau - \tau') = \delta(x - x')G^{jj'}(\tau, \tau')$ is a convenient notation for the non-interacting phonon propagator and $\mathcal{T}$ indicates Euclidean time-ordering. After Fourier transforming to (k, q, ω_n) coordinates and performing the analytic continuation $i\omega_n \to \omega$ we obtain the desired retarded phonon Green's function

$$D(k, q, \omega) = G(q, \omega) + g^2 G^2(q, \omega)\chi(k, q, \omega), \tag{39}$$

where $G(q, \omega) = \frac{a}{m} \frac{1}{-\omega^2 + \omega(q)}$ is the bare phonon Green's function and $\chi(k, q, \omega)$ stems for the Fourier transform of the retarded correlator of $: \cos(\sqrt{2\pi}\phi^j) :$. In order to evaluate bulk corrections arising from inter-chain coupling, we will calculate this correlator using a RPA approach in the interchain interaction[12]. It reads

$$\chi^{RPA}(k, q, \omega) = \frac{\chi^0(k, \omega; T)}{1 - g^2 G_{inter}(q, \omega)\chi^0(k, \omega; T)}, \tag{40}$$

where $\chi^0(k, \omega; T)$ is the already known finite temperature one chain $: \cos(\sqrt{2\pi}\phi) :$-correlator and G_{inter} is the inter-chain bare phonon propagator, defined in coordinate space by the subtraction

$$G_{inter}^{j-j'}(x - x', \tau - \tau') = G^{j-j'}(x - x', \tau - \tau') - \delta^{jj'} G^0(x - x', \tau - \tau'). \tag{41}$$

The one chain $: \cos(\sqrt{2\pi}\phi) :$-correlator at finite temperature has been computed elsewhere[1,6,18], being given by

$$\chi^0(k, \omega; T) = \frac{2d}{T} I_1\left(\frac{(\omega - \Delta)}{2\pi T}\right) I_1\left(\frac{(\omega + \Delta)}{2\pi T}\right), \tag{42}$$

where $d \sim 0.37$ is a constant weakly depending of the momentum cutoff in the bosonization procedure, $\Delta = v_F|k - \pi|$ is the lower edge of the two spinon continuum, and

$$I_1(k) = \frac{1}{2\pi} \int_0^\infty dx e^{ikx}(\sinh(x))^{-\frac{1}{2}} =$$
$$\frac{1}{2\sqrt{2\pi}} \frac{\Gamma[\frac{1}{4} - i\frac{k}{2}]}{\Gamma[\frac{3}{4} - i\frac{k}{2}]}. \tag{43}$$

It will be useful to note that at low frequency one can expand

$$T\chi^0(k,\omega;T) \approx \chi_0 - i\chi_1\frac{\omega}{2\pi T} + \chi_2\left(\frac{\omega}{2\pi T}\right)^2,\tag{44}$$

with $\chi_0 \sim 0.26$ and $\chi_2 \sim 2.2$.

The Fourier transform of the interchain propagator G^{inter} is obtained (see Section II) as

$$G^{inter}(q,\omega) = \frac{1}{-\omega^2 + \omega(q)} - \Upsilon(\omega),\tag{45}$$

with

$$\Upsilon(\omega) = \frac{1}{2\pi}\int\frac{dq'}{\omega^2(q') - \omega^2} = \frac{1}{\sqrt{(\omega_\parallel^2 - \omega^2)}\sqrt{(\omega_\parallel^2 + \omega_\perp^2 - \omega^2)}}.\tag{46}$$

We are interested in the temperature evolution of the SP active phonon mode, given by $k = \pi$ and $q = 0$. From eq.(39-45) we have

$$D(0,\pi,\omega) = \frac{g^2(1 - g^2\Upsilon(\omega)\chi^0(\pi,\omega;T))}{G^{-1} + \frac{g^2}{2}(1 - G^{-1}\Upsilon(\omega))\chi^0(\pi,\omega;T)}\tag{47}$$

and the phonon frequencies are given by the poles over the real axis of this expression, *i.e.* the roots of the following equation

$$-\omega^2 + \omega_\parallel^2 + \frac{g^2}{2}(1 - (\omega_\parallel^2 - \omega^2)\Upsilon(\omega))Re\chi^0(\pi,\omega;T) = 0.\tag{48}$$

Let us start the analysis of the consequences of the previous results by recalculating the spin-Peierls transition temperature. Note that, different than the previous Section, we are now coming from the high temperature phase to the transition point. As discussed by GW, T_{SP} is signaled by a macroscopic occupation of the Peierls active phonon mode, *i.e.* the transition temperature takes place when eq. (48) has a solution $\omega = 0$. We then obtain

$$T_{SP} = \frac{\chi_0 g^2}{2\omega_\parallel^2}\left(1 - \frac{1}{\sqrt{1 + \frac{\omega_\perp^2}{\omega_\parallel^2}}}\right).\tag{49}$$

It is important to stress that eq. (49) gives the same dependency of T_{SP} on the microscopic parameters than eq. (33) in the previous Section; differences in the numerical prefactor arise from different criteria to fix the momentum cutoff. Note however that relation (34) is fulfilled. This results prove that our RPA procedure contains the previous MF approach when the static properties are considered.

In the rest of this Section we face the question of phonon softening, discussing the calculation of the renormalized phonon frequencies. We use (49) to eliminate the cut-off dependent coupling g^2 from eq. (48). After straightforward algebra we obtain

$$\chi_0\left(1 - \frac{1}{\sqrt{1 + (\frac{\omega_\perp}{\omega_\parallel})^2}}\right)\left(\left(\frac{\omega}{\omega_\parallel}\right)^2 - 1\right)/\left(1 - \frac{\sqrt{1 - (\frac{\omega}{\omega_\parallel})^2}}{\sqrt{1 + (\frac{\omega_\perp}{\omega_\parallel})^2 + (\frac{\omega}{\omega_\parallel})^2}}\right) = T_{SP}Re\chi^0(\pi,\omega).\tag{50}$$

This equation is the generalization of the GW results to finite values of $\frac{\omega_\perp}{\omega_\parallel}$, and agrees with their corresponding eq. (6) when $\frac{\omega_\perp}{\omega_\parallel} \gg 1$. There are two different temperature dependence regimes of the renormalized phonon frequency $\omega(\pi,0)$, as depicted in Fig. 2. For low enough $\omega_\parallel$ the phonon progressively softens from higher T until T_{SP}, where it drops to zero frequency. In this regime the phonon softening explains the SP transition. For higher $\omega_\parallel$, the phonon frequency remains finite up to the SP temperature and no soft phonon behavior is obtained; in fact, there can be partial softening or even hardening of the renormalized frequency close to T_{SP}. However, an additional solution $\omega = 0$ in eq. (50) signals the appearance of a central peak in the dynamical structure factor, leading to the SP transition[6].

The limiting value of $\omega_\parallel/T_{SP}$ for separation of regimes depends on $\omega_\perp$. To find this transition analytically it is enough to compare concavities of both sides of eq. (50) at $T = T_{SP}$, as seen in Fig. 2. Expanding both sides up
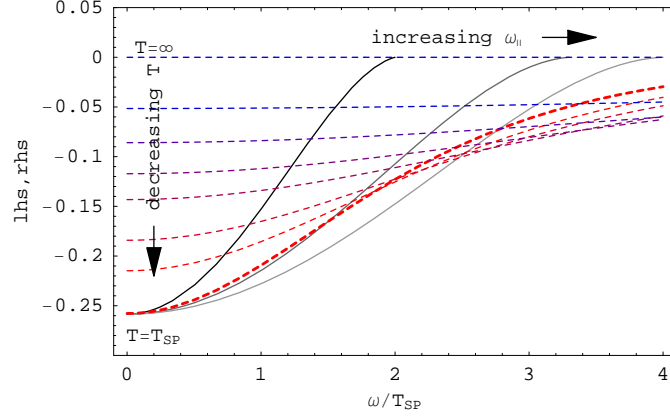
FIG. 2: Evolution of the SP relevant phonon mode. Dashed lines, from blue to red, represent the rhs of eq. (50) when temperature is lowered until T_{SP}. Solid gray lines represent the lhs for $\omega_\parallel/T_{SP} = 2, 3, 4$ and $\omega_\perp/T_{SP} = 1$. The intersections illustrate the evolution of the renormalized phonon frequency. For $\omega_\parallel/T_{SP} = 2$ the phonon softens completely, for $\omega_\parallel/T_{SP} = 3$ it softens partially, and for $\omega_\parallel/T_{SP} = 4$ it hardens close to T_{SP}.

to second order in $\frac{\omega}{T_{SP}}$, the soft phonon regime is reached when, at $T = T_{SP}$, the coefficient of ω^2 in the r.h.s. is smaller than the one in the l.h.s. Under this condition the bare phonon frequency (that obtained at hight T) evolves continuously to zero when the temperature is lowered until the transition temperature. The following inequality should then be fulfilled to have the soft phonon regime:

$$\frac{\omega_\parallel}{T_{SP}} < 2\pi \sqrt{\frac{\chi_0}{\chi_2}} \sqrt{1 + \frac{1}{2} \frac{(1 + \sqrt{1 + (\omega_\perp/\omega_\parallel)^2})}{1 + (\omega_\perp/\omega_\parallel)^2}}. \tag{51}$$

In the other case, the bare phonon frequency evolves to some finite value at the SP transition. In Fig. 3 we show the phase diagram of the spin-phonon system on the $\omega_\perp - \omega_\parallel$ plane. Note that in a wide range of high enough $\frac{\omega_\perp}{T_{SP}}$ the separatrix is given by $\frac{\omega_\parallel}{T_{SP}} \sim 2.2$ as in GW. Our result extends this condition for finite values of $\frac{\omega_\perp}{T_{SP}}$ where realistic spin-Peierls materials as $CuGeO_3$ live. This also explains why the RPA approach for the spin-phonon coupling underlying the GW calculation compares well with experiments on $CuGeO_3$.

In Fig. 4 we show the temperature dependence of the renormalized phonon frequency for $\frac{\omega_\perp}{T_{SP}} = 1$ where the phase diagram of Fig. 3 is not completely flat. The behavior shifts from a soft to a non soft phonon regime at some intermediate value of $\frac{\omega_\parallel}{T_{SP}}$. In this last regime the mechanism of the SP transition has been associated with the emergence of a central peak in the spectral signal measured in neutron scatering experiments[22]. For high enough $\frac{\omega_\parallel}{T_{SP}}$ the phonon hardens from a minimum value at some intermediate temperature. At $T = T_{SP}$ the frequency of the phonon is the bare one as in the high temperature limit. We will use this fact to fix $\omega_\parallel$ for $CuGeO_3$. Note that the T-dependence of the phonon is similar to the one obtained by GW but the frequency and temperature scale are different.

From the previous results we can follow the T-dependence of the Peierls active phonons in $CuGeO_3$. In Fig. 4 (b), we show our prediction for the higher energy mode T_2^+, which is the most anomalous and strongly coupled to the magnetism[4]. We take as a bare phonon frequency $\omega_\parallel = 6.8 THz$ i.e. its low temperature value. For $\omega_\perp$ we use the relationship obtained in the previous Section. Note that a value of $T_{SP} = 14.1K(0.294THz)$ has been used to give the frequencies in Thz and the temperatures in K. Our results compare well with Fig. 3 of [4]. In fact we predict a stronger hardening than the one experimentally observed (7% against 4.5% seen in the experiment). This could be due to the simplified model we use, which does not take into account the fact that two phonon modes are necessary to describe the SP transition in $CuGeO_3$[4].

Besides, we can make a prediction for the phonon frequency behavior at higher temperature than the one already measured. It should increase as shown in Fig. 4, approaching the bare frequency at very high T. We note that at room temperature the phonon frequency does not correspond to the bare one as expected. It is almost the minimum of the predicted phonon frequency. The bare frequency is only obtained at $T = T_{SP}$ and at very high temperature (probably not experimentally accessible).

To summarize the results of the present Section, we have generalized the MF approach of the previous Section to the dynamical correlation functions in the high temperature phase. Our approach relies on a RPA on the effective interchain coupling generated by the spin-phonon interaction. In contrast to the previous theoretical calculations,
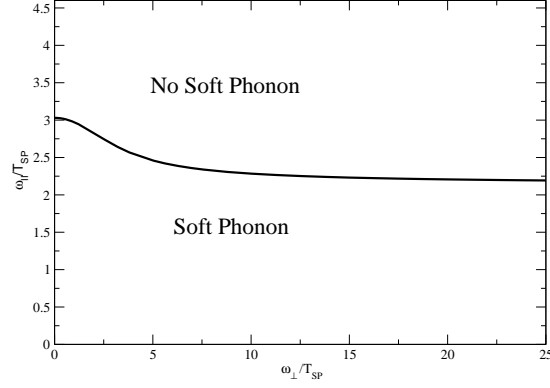
FIG. 3: The line separating the zone in the $\frac{\omega_\perp}{T_{SP}}$, $\frac{\omega_\parallel}{T_{SP}}$ plane, where the spin-Peierls transition takes place by softening of the phonon from the one where the Peierls active phonon does not soften completely.
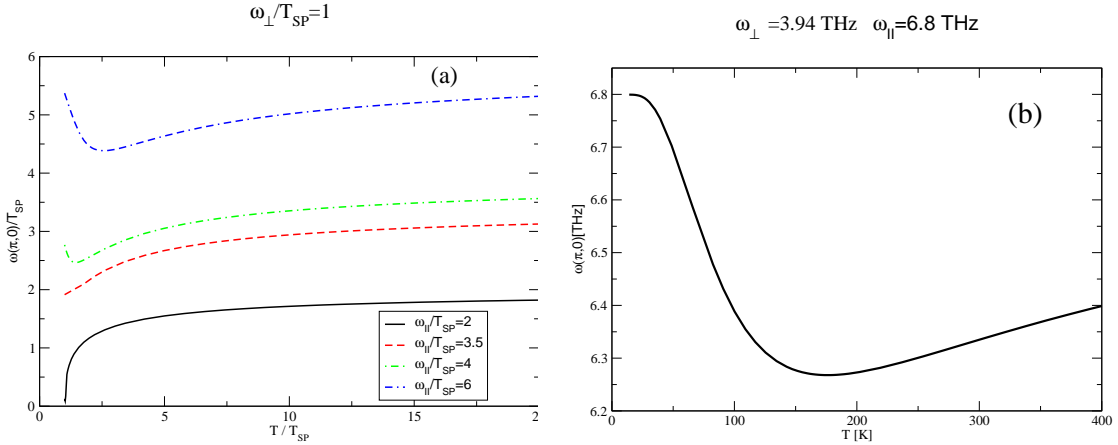

FIG. 4: (a)The temperature dependence of the renormalized phonon frequency for different values of the bare $\frac{\omega_\parallel}{T_{SP}}$, with $\frac{\omega_\perp}{T_{SP}} = 1$ (b) The hardening of the phonon for the parameters describing the higher energy active SP mode in $CuGeO_3$. The bare values used for $\omega_\parallel$ and $\omega_\perp$ are shown on top of the Figure.

the present one does not presuppose the existence of a soft phonon mode in the non magnetic regime. Therefore, it can been applied to $CuGeO_3$. Moreover, the qualitative behavior of the Peierls active phonon is similar to the one previously obtained. There is a regime corresponding to low frequency phonon where the structural phase transition takes place by progressive softening of a phonon from the high temperature phase. For higher bare phonon frequency no soft phonon is observed and it can even harden from the room temperature value to the transition temperature one. This is precisely the behavior seen in neutron scattering measurements of the phonon spectra in $CuGeO_3$.

V. CONCLUSIONS

We have developed a route for the spin-Peierls transition which goes beyond the usual adiabatic treatment of the phonon field. We emphasized the essential character that plays the dispersion of the phonon in the transversal direction to the magnetic chains. Moreover, the results of the present paper show that, when the adiabatic hypothesis for the phonon coordinates is relaxed, the one-chain model does not represent a good starting point to describe a real system. Furthermore the effective interchain interaction generated by the phonons is an essential ingredient for the opening of the gap and the existence of a finite temperature phase transition. The precise determination of the SP transition temperature from the microscopic parameters strongly depends on the width of the transversal phonon dispersion.

Our approach for the dynamics of the phonon mode in the high temperature phase justifies and generalizes previous calculations of the phonon spectra based on the Cross and Fisher early work. Applied to $CuGeO_3$, we show that

the phonon does not soften until the phase transition. Moreover the overall temperature dependence of the phonon frequency is consistent with experimental determinations.

As the elastic interaction between the chains play a central rol in non-adiabatic spin-Peierls systems, we anticipate that a change in the relative positions of the magnetic ions in different chains will change the phase diagram and the mechanism of the phase transition. In this sense it is highly interesting to study the recently discovered quasi-one-dimensional magneto-elastic system TiOCl with an intermediate incommensurate phase where the Ti ions are not aligned in the direction perpendicular to the magnetic chain[3]. We will study in a forthcoming work this system within the formalism developed in the present paper.

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